Supporting material (ESI) for PCCP

First-Principles Study of the Formation and Migration of Native Defects in LiNH₂BH₃

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Figure S1. The left panel contains the calculated band structure of the ground state of LiNH₂BH₃. The right panel is the complete electron density of states, in arbitrary units.
Figure S2. The energy profiles for the migration of $V_{(B)H}^+$ and $V_{(N)H}^-$. 
Figure S3. The energy profiles for the migration of $I^+_H$ and $I^-_H$. 
Figure S4. The energy profiles for the migration of neutral H$_2$ interstitial along [100] and [001] direction.
Figure S5. The energy profiles for the migration of $I_{Li}^-$ and $V_{Li}^-$. 